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Numerical Computation of Hydrodynamic Flows Which Contain a Shock

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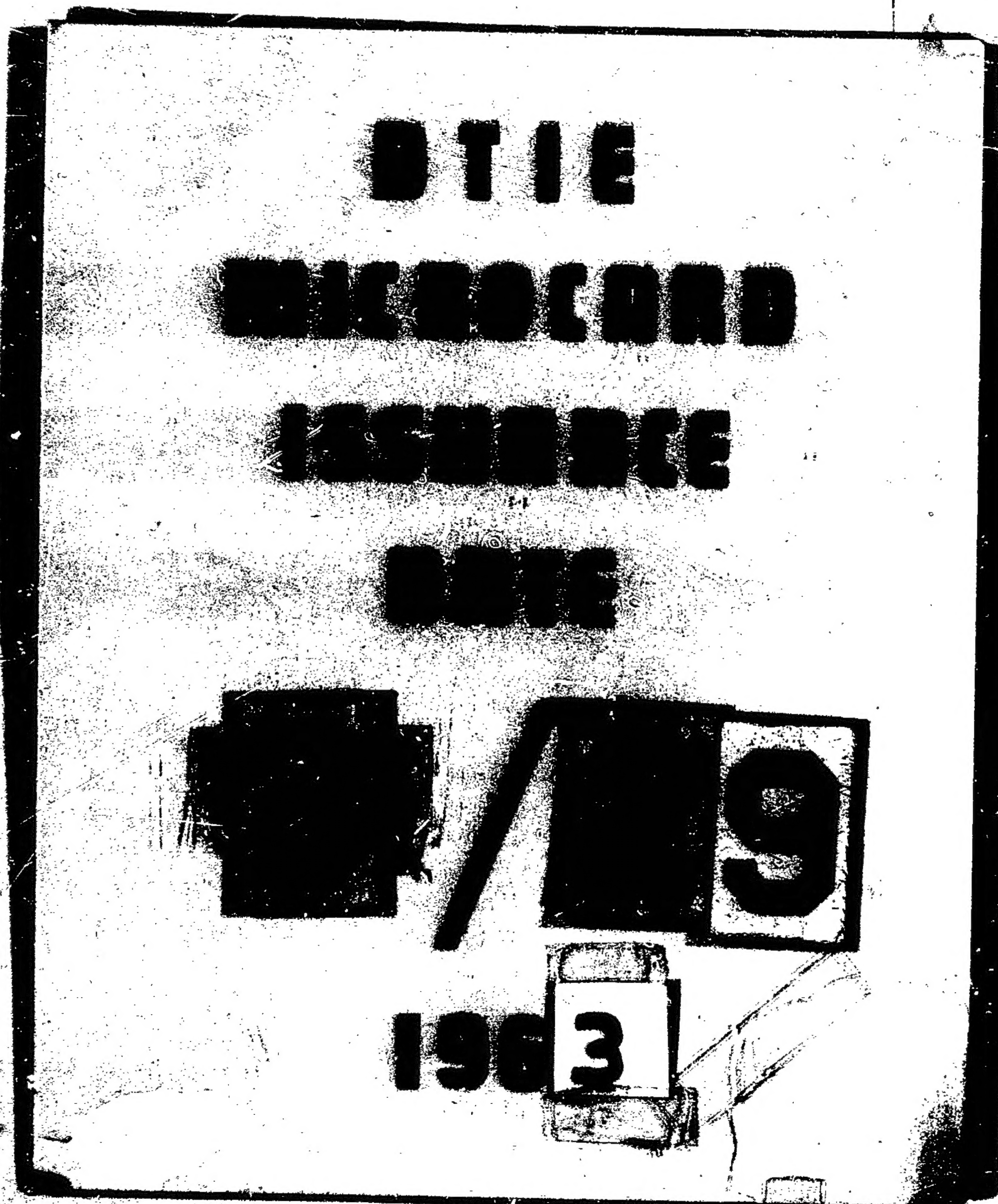

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NUMERICAL COMPUTATION OF HYDRODYNAMIC FLOWS WHICH CONTAIN A SHOCK

by

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ABSTRACT

Professor R. D. Richtmyer has described a finite difference method for the computation of hydrodynamic flows which contain a shock [3,4]. This method uses the Eulerian form of the hydrodynamic equations, is explicit, is of second order accuracy, and is based on shock fitting rather than the introduction of artificial viscosity. This paper describes the result of numerical computations using a modification of this finite difference method. The method is applied to a one-dimensional problem for which a solution can be computed by solving an ordinary differential equation. Therefore we are able to determine the accuracy of the method for this problem.

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NUMERICAL COMPUTATION OF HYDRODYNAMIC FLOWS WHICH CONTAIN A SHOCK

1. Introduction.

Our objective is to test the method of Richtmyer for stability and accuracy by using it to compute the one-dimensional flow of a shock down a tube. The shock fitting scheme is a slight modification of that proposed by Richtmyer [3,4]. Two finite difference schemes for the flow behind the shock are described and tested. We will describe the problem used for the test calculation, the finite difference methods, and then the results of the calculations performed on the IBM 7090.

2. Description of the Problem.

The problem for which we will compute the solution is that of a shock moving down a tube with a variable density cold gas ahead of the shock. This problem was suggested by Professor Peter Lax. It has the advantage of providing an exact solution with a shock of variable strength. The problem and its solution is due to J. Keller [1]. We denote the distance along the tube by x and the pressure, density and velocity ahead of the shock by P_o, ρ_o, and u_o, respectively. Keller showed that if $P_o = u_o = 0$ and

$$\rho_o = 2F_o(\gamma+1)^{-1}R_o^2 x^{-1}\left[\frac{2\alpha_1}{1-\gamma} R_o^2 + \alpha_2 R_o^{\frac{4}{\gamma+1}} x^{\frac{2(\gamma-1)}{\gamma+1}}\right]^{-\frac{3}{2}}$$

then the flow behind the shock can be determined by solving the following differential equation

$$J'(t) = \left[\frac{2\alpha_1}{1-\gamma} J(t)^{(1-\gamma)} + \alpha_2\right]^{\frac{1}{2}} .$$

In the above equations F_o, R_o, α_1, and α_2 are arbitrary constants and γ is the ratio of specific heats. If we define the function $F(x)$ by

$$F(x) = F_o x \left[\frac{2\alpha_1 R_o^2}{1-\gamma} + \alpha_2 x^2\right]^{-\frac{1}{2}} ,$$

then the flow behind the shock is given by

$$\rho(t,x) = -\frac{F'(xJ^{-1}(t))}{\alpha_1 x} \quad P(t,x) = J^{-\gamma}(t)F(xJ^{-1}(t))$$

$$u(t,x) = xJ'(t)J^{-1}(t).$$

The shock position is given by $R(t) = R_o \left[J(t)\right]^{\frac{\gamma+1}{2}}$. In our computations we use the values $F_o = 50$, $R_o = 0.0868$, $\alpha_1 = -1$, $\alpha_2 = 0.195$, and $\gamma = 3$. In figure 2 graphs of $p(0,x)$, $\rho(0,x)$, and $u(0,x)$ are shown. The function $J(t)$ is evaluated by a Runge-Kutta routine; or if $\gamma = 3$, then the differential equation for $J(t)$ is solved by an explicit formula. The flow is computed by the finite difference scheme between $x = a$ and the shock. The boundary conditions at $x = a$ are obtained from the exact solution described above. The flow is then determined from the usual hydrodynamic equations behind the shock and the Hugoniot relations for the shock.

3. <u>The Finite Difference Equations</u>.

We denote the energy and momentum by e and m, respectively and make the definitions

$$v = \begin{bmatrix} \rho \\ e \\ m \end{bmatrix} \qquad f(v) = \begin{bmatrix} m \\ \frac{\gamma m e}{\rho} - \frac{\gamma-1}{2}\frac{m^3}{\rho^2} \\ (\gamma-1)e - \frac{\gamma-3}{2}\frac{m^2}{\rho} \end{bmatrix}$$

The flow equations in conservation form are

$$\frac{\partial v}{\partial t} + \frac{\partial f}{\partial x} = 0 \quad \text{or} \quad \frac{\partial v}{\partial t} + A\frac{\partial v}{\partial x} = 0$$

where A is the Jacobian of $f(v)$. Two finite difference schemes are tested on this problem. The first is the scheme of Lax and Wendroff [2] and the second is an iterative scheme to be described below.

The difference equations used by Lax and Wendroff are the following:

$$v_i^{n+1} = v_i^n - \frac{\lambda}{2}(f_{i+1}^n - f_{i-1}^n) + \frac{\lambda^2}{2}\left[A_i^n(f_{i+1}^n - f_i^n) - A_{i-1}^n(f_i^n - f_{i-1}^n)\right] ,$$

where $\lambda = \frac{\Delta t}{\Delta x}$, $v_i^n = v(t_n, x_i)$ and similarly for A_i^n and f_i^n. These equations are based on an expansion of $v(t,x)$ in powers of Δt about $(t_n + \frac{\Delta t}{2})$. Using the flow equations, we find the first two terms of the expansion to be

$$\left\{\frac{\partial v}{\partial t}\right\}^{n+\frac{1}{2}} = -\left\{\frac{\partial f}{\partial x}\right\}^n + (\Delta t)\left\{\frac{\partial(A\frac{\partial v}{\partial x})}{\partial x}\right\}^n .$$

A stability analysis by von Neumann's method indicates that this scheme is stable provided that $\lambda < \frac{1}{|a|}$ where a is the largest eigenvalue (in absolute value) of any of the matrices A_i^n. This analysis is based on the linearized equations and ignores the influence of the boundary conditions. The truncation error in v_i^n is $O(\Delta x^3)$.

We denote the mesh point immediately behind the shock by x_{is} and denote the shock position by $R^n = R(t_n)$ (strictly speaking $is = is(n)$, see figure 1). The above difference equations can not be used at x_{is} since x_{is+1} does not lie behind the shock. In order to compute $\partial f/\partial x$ with second order accuracy we must use the values of v at three points. We can use the points x_{is-2}, x_{is-1}, and x_{is} or x_{is-1}, x_{is} and R^n. The results of the computation show that the first choice is somewhat better, although the difference is not significant. The difference equations at x_{is} are, using the first choice,

$$v_{is}^{n+1} = v_{is}^n - \frac{\lambda}{2}(f_{is-2} - 4f_{is-1} + 3f_{is})$$

$$+ \frac{\lambda^2}{2}\left[A_{is}^n(f_{is}^n - f_{is-1}^n) - A_{is-1}^n(f_{is-1}^n - f_{is-2}^n)\right] .$$

The second finite difference scheme is an iterative scheme defined by

$$\omega_i^o = v_i^n$$
$$v_i^{n+1} = \omega_i^p$$
$$\omega_i^{s+1} = v_i^n - \frac{\lambda}{4}\left[f(\omega_{i+1}^s) - f(\omega_{i-1}^s) + f(v_{i+1}^n) - f(v_{i-1}^n)\right] .$$

This scheme is described in more detail elsewhere [5]. The scheme is stable if $\lambda < 2/|a|$ and $p = 3,4,7,8,\ldots$ and unstable otherwise. (a is the largest eigenvalue, (in absolute value, of any of the matrices A_i^n.) When $i = is$ we must modify the difference quotients in the same manner that they were modified in the Lax-Wendroff scheme. If $p \geq 2$, then the truncation error is $O(\Delta x^3)$.

4. The Shock Fitting Method.

The shock fitting method is essentially that proposed by R. D. Richtmyer [3]. We let ρ_s, e_s, m_s denote values immediately behind the shock and let V denote the velocity of the shock. Thus there are four unknowns at the shock. The Hugoniot relations provide three equations relating these unknowns at the shock. The three flow equations must provide the additional relation. Only one of the three characteristics at the shock lies behind the shock. Richtmyer proposed the use of the corresponding characteristic equation as the fourth relation. He also conjectured that the use of a characteristic equation corresponding to a characteristic lying ahead of the shock would lead to instability. This conjecture is tested and it is correct.

This characteristic equation can be written as follows

$$r \cdot \frac{\partial v}{\partial t} = - r \cdot \frac{\partial f}{\partial x} = - r \cdot A\frac{\partial v}{\partial x} = - ar \cdot \frac{\partial v}{\partial x}$$

where A is the Jacobian of $f(v)$ and r is the eigenvector of A corresponding to the eigenvalue $a = u + c$ $(c = \sqrt{\gamma p/\rho})$.

The Hugoniot relations can be written as

$$V(v_s - v_o) = f(v_s) - f(v_o) = f_s - f_o .$$

The shock fitting is done by iteration. It is the same regardless of which scheme is used for the flow behind the shock (that is, Lax-Wendroff or iteration). We assume that approximations for v_s^{n+1} and V^{n+1} are known, then we compute corrected values $\bar{v}_s^{n+1} = v_s^{n+1} + \Delta v$ and $\bar{V}^{n+1} = V^{n+1} + \Delta V$ as follows.

If we denote the directional derivative along the shock by D/Dt, then

$$\frac{Dv}{Dt} = \frac{\partial v}{\partial t} + V\frac{\partial v}{\partial x} .$$

From the characteristic equation we have

$$r \cdot \frac{Dv}{Dt} = - r \cdot (A - VI)\frac{\partial v}{\partial x} .$$

The above equation in finite difference form and the Hugoniot relations are ($\left\{\frac{\partial v}{\partial x}\right\}_s^{n+\frac{1}{2}}$ must be evaluated by a difference quotient, which will be defined below)

$$r_s^{n+\frac{1}{2}} \cdot (\bar{v}_s^{n+1} - v_s^n) = - \Delta t\, r_s^{n+\frac{1}{2}} \cdot (A_s^{n+\frac{1}{2}} - V_s^{n+\frac{1}{2}} I) \left\{\frac{\partial v}{\partial x}\right\}_s^{n+\frac{1}{2}}$$

$$\bar{V}^{n+1}(\bar{v}_s^{n+1} - v_o) = f(\bar{v}_s^{n+1}) - f(v_o).$$

Expanding these equations out to the first order in Δv and ΔV we have (let $r = r_s^{n+\frac{1}{2}}$, $J = \{A - VI\}_s^{n+1}$

$$r \cdot \Delta v = r \cdot v_s^n - \Delta t \{a - V\}_s^{n+\frac{1}{2}} r \cdot \left\{\frac{\partial v}{\partial x}\right\}_s^{n+\frac{1}{2}} - r \cdot v_s^{n+1}$$

$$\Delta v = J^{-1}\left\{V(v_s - v_o) - (f - f_o)\right\}^{n+1} + \Delta V J^{-1}\left\{v_s - v_o\right\}^{n+1} .$$

These equations are easily solved for ΔV and Δv. The average values $\{\ \}^{n+\frac{1}{2}}$ are determined from v^{n+1}, v^n, V^{n+1}, and V^n and are therefore independent of Δv and ΔV.

The value of $\left\{\frac{\partial v}{\partial x}\right\}_s^{n+\frac{1}{2}}$ is $\left\{\frac{\partial v}{\partial x}\right\}_s^{n+\frac{1}{2}} = \frac{1}{2}\left[\left\{\frac{\partial v}{\partial x}\right\}_s^{n+1} + \left\{\frac{\partial v}{\partial x}\right\}_s^{n}\right]$. The latter derivatives must be computed to second order accuracy in Δx. Two methods of computation are tested. The first is to pass a second degree polynomial through the values of v^{n+1} (or v^n) at the points x_{is-1}, x_{is} and R^{n+1} (or R^n). The second is to fit a second degree polynomial by least squares through the values of v^{n+1} (or v^n) at the points x_{is-2}, x_{is-1}, x_{is} and R^{n+1} (or R^n). The first method is satisfactory, the second is not (see the discussion of the results below).

Thus we have an iterative method for computing the solution at the shock. If the iterative scheme is used for the flow behind the shock, then one iteration at the shock is performed for each iteration behind the shock. If the Lax-Wendroff scheme is used behind the shock, then the solution behind the shock is computed before the iterations are performed at the shock. In the Lax-Wendroff scheme three iterations are generally used in the shock fitting.

We must still describe how this scheme computes the solution at a mesh point which is overtaken by the shock, for example the

point (t_{n+1}, x_{is+1}) in figure 1. It would obviously be awkward to use the flow equations to compute the solution at this point; therefore interpolation is used. A second degree polynomial is passed through the values of v^{n+1} at the points x_{is-1}, x_{is} and R^{n+1} and this polynomial is used to interpolate for v^{n+1}_{is+1}. This is the same polynomial used to compute $\left\{\frac{\partial v}{\partial x}\right\}^{n+1}_{s}$. We could also use a polynomial obtained by a least squares fit. However, this least squares fit is also unsatisfactory.

The value of Δt is changed at each time-step according to the formula $\Delta t = \frac{\beta \Delta x}{a_m}$ where $a_m = |u_s + c_s|$, $c_s = \sqrt{\gamma P_s/\rho_s}$ and $0 < \beta < 1$. Usually we take $\beta = 0.9$. The program will stop if the shock overtakes more than one mesh point per time-step.

5. The Results of the Calculation.

The tables below show the maximum percentage error in the pressure after 20, 40, and 100 time-steps for various values of Δx. Unless otherwise stated the least squares fit was not used to compute the derivatives or to interpolate for the overtaken mesh point. Also, unless otherwise stated $\Delta t = 0.9\Delta x/a_m$.

Table I. Percentage error for the Lax-Wendroff method.

Δx	Time-steps 20	40	100
.05	0.17	0.32	0.69
.025	0.022	0.043	0.098
.0125	0.0029	0.0055	0.013

Table II. Percentage error for the iteration method.

Δx	Time-steps 20	40	100	200	No. of Iterations
0.05	0.17	0.32	0.69	--	3
0.025	0.025	0.046	0.098	--	3
0.0125	0.0049	0.0075	0.014	--	3
0.05	0.16	0.32	0.69	--	4
0.05	0.32	0.41	0.76	1.20	2

Note that there is very little difference in the accuracy of the two methods. Inspection of these results shows that the error is approximately $O(\Delta x^3)$ especially for the Lax-Wendroff method.

Also note that the iteration method shows no sign of instability out to 200 time-steps when only two iterations are used. This in spite of the stability analysis which indicates instability for two iterations. This is probably due to the fact that $\Delta t = 0.9\Delta x/a_m$ where the maximum allowable value of Δt for the iteration method is $\Delta t = 2\Delta x/a_m$. If the larger value of Δt is used the shock will overtake two mesh points per time-step. Other experiments with the iteration scheme have indicated instability when $\Delta t = 1.9\Delta x/a_m$ and apparent stability with $\Delta t = 0.9\Delta x/a_m$ when only two iterations are used [5].

Table III. Percentage error for the Lax-Wendroff method when the difference equation for v^{n+1}_{is} uses the values of v^n at x_{is-1}, x_{is}, and R^n (see section 3).

Δx	Time-steps 20	40	100
0.05	0.25	0.31	0.69
0.025	0.031	0.043	0.098

Comparison with table 1 shows that slightly better results are obtained using the values at x_{is-2}, x_{is-1}, and x_{is} in the difference equation for v_{is}^{n+1}. In this case the values of v on the shock are never used in the computation of the flow behind the shock. When the shock overtakes a mesh point the values of v on the shock are used in the interpolation for the overtaken mesh point. This is the only way the values on the shock can influence the flow behind the shock.

Table IV. Percentage error when a least squares fit is used to compute $\left\{\frac{\partial v}{\partial x}\right\}_s$ and is used in the interpolation. The Lax-Wendroff scheme was used for the flow behind the shock.

Δx	Time-steps 20	40	100
0.05	0.98	0.28	0.66
0.025	0.10	0.40	1.8

Table V. In this case the shock fitting used the equations expressed in terms of p, ρ and μ rather than ρ, ξ, and m. These equations are described in the report by Richtmyer [3]. Otherwise conditions are the same as in IV above.

Δx	Time-steps 20	40	100
0.05	0.17	0.27	0.59
0.025	8.0	8.5	9.0
0.0125	0.12	0.34	0.26

Table VI. In this case conditions are the same as in V except that the least squares fit is not used for interpolation.

Δx	Time-steps 20	40	60	80	100
0.025	0.04	0.19	0.06	1.5	0.39
0.0125	0.01	0.01	0.01	0.01	0.01

Note the sudden jump in the error at 80 time-steps. It is clear that the least squares fitting is unsatisfactory.

These computations were carried out on the IBM 7090 at New York University. The author wishes to thank Professor Richtmyer for suggesting this problem.

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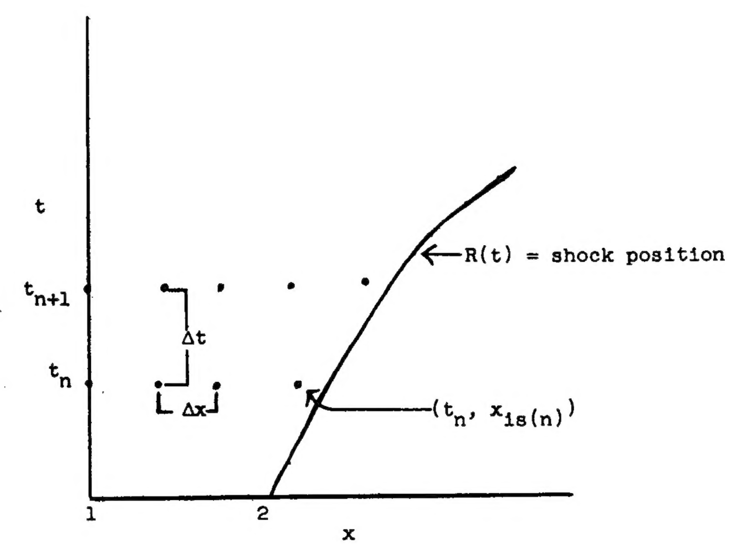

Figure 1. The shock fitting method.

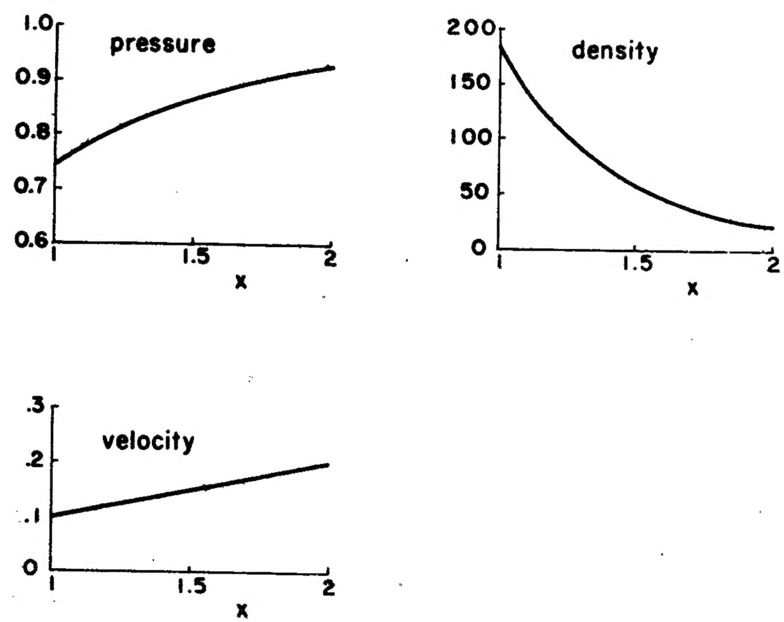

Figure 2. The initial values of p, ρ and μ.